ABSTRACT

Aluminum is the most abundant metal in the Earth's crust and it has high enthalpy of combustion. It is therefore used in various propulsion and energy conversion applications. One of the main concern is high ignition temperatures of micro aluminum particles. As the size of the particle decrease form microscale to nanoscale, particle possesses distinct properties at nanoscale due to increase in the fraction of surface atoms. Nano aluminum particles have the lower ignition temperatures. One of the ignition theory predicts that ignition of nanoparticles take place upon the melting of aluminum core. As the melting is size dependent at nanoscale, it is necessary to study the size effect on melting point of aluminum nanoparticles. Molecular dynamics simulations are carried out to observe the size effects on the melting point of different shapes chosen based on the various practical applications. The atomic interactions are defined using Embedded atom method (EAM) potential. Melting point is characterized using different thermophysical and structural properties like potential energy per atom, density and mean square displacements (MSD). The average properties are not able to detect the onset of melting point clearly because it reduces the contribution of surface atoms. It is therefore required to observe the radial variation of properties to determine the onset of melting point. Melting of nanocrystals take place heterogeneously in every case means, the melting start form the surface and reaches to the core and it is apparent by observing the potential energy of different bins. Various thermodynamic melting models predict the size dependence of the melting point of nanocrystals but these models require some thermophysical parameters as input. These parameters include bulk melting point, latent heat of melting, solid density and surface free energy of solid and liquid. These parameters are calculated using molecular dynamics simulation and fed to thermodynamic models. Predictions of the thermodynamic models are compared

with the predictions of the MD simulations. It is observed that melting point of the nanospheres and nanocubes decrease suddenly after 4 nm size and nanofilms don't show much depression of melting point. The Surface free energy of the solid-vapor interface depends on the orientation of the surface which leads to the different melting point corresponding to different orientations which is also shown using molecular dynamics simulations. Model predictions are qualitatively comparable with the melting points obtained using MD.